Diffraction grating efficiency calculations based on real groove profiles

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Introduction

- The program we are attempting to bring about combines 3 difficult features, in order to demonstrate accuracy of efficiency predictions:
  - 1 -- Accurate groove metrology methods on surface relief gratings
  - 2 -- Rigorous and usable electromagnetic efficiency calculation codes
  - 3 -- Accurate efficiency measurements in polarized light

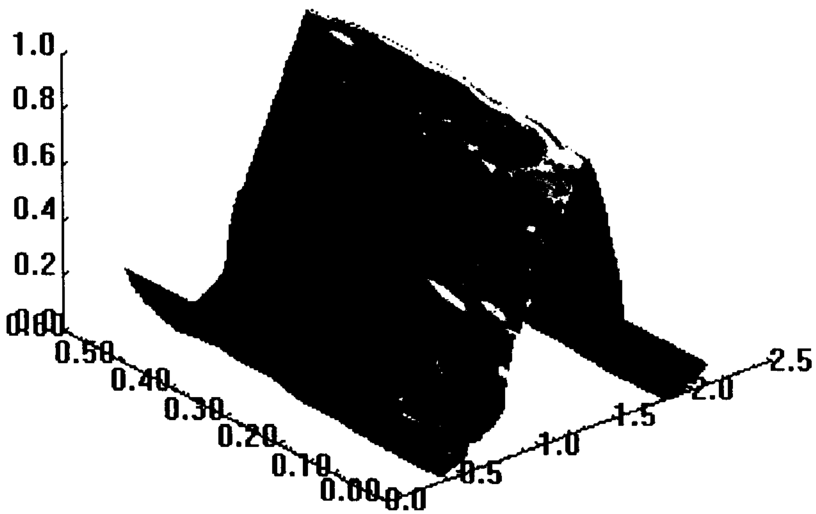
- The benefit would be an increase in yield for high-performance gratings. Many such applications suffer long lead time or serious performance loss when new gratings are made which do not meet requirements or expectations.

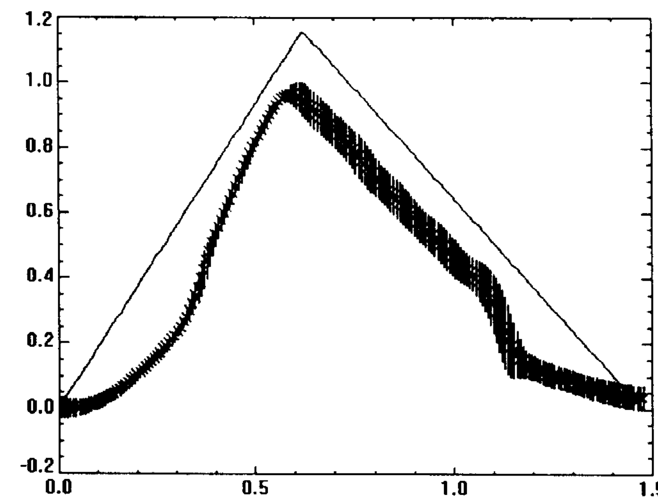
AFM groove metrology

- Returns images with high fidelity to $\geq$ 20 nm lateral features
  - Note - many other methods exist; For $h/d < 0.5$, $0.1 \leq d\ (\mu m) \leq 50$, this is the best method. Most gratings for X-ray to IR spectroscopy are in this regime.

- Pushes hard on calibration issues:
  - Height calibration
  - Height linearity
  - (for fine pitch gratings) Tip convolution effects
  - Lateral calibration (but usually know spacing d)
  - AFM tip noise (for smooth gratings)

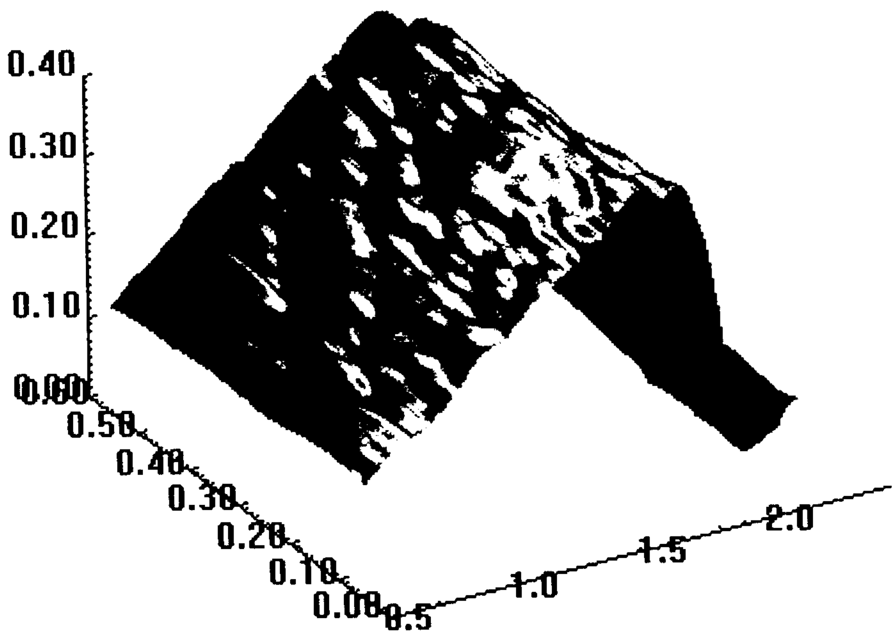
AFM groove image example 1 [micron units]

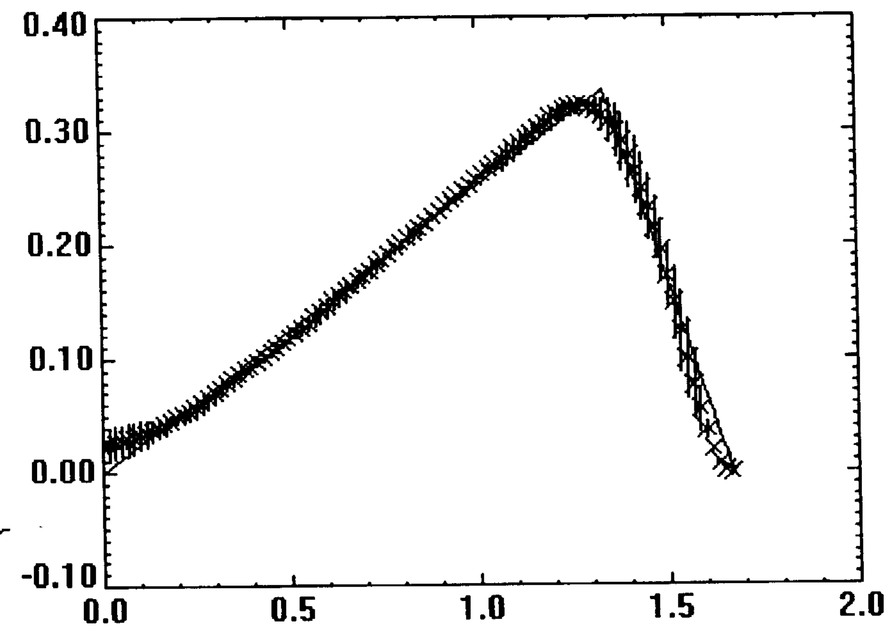




- 720/mm transmission grating, steep blaze ~ 43 degrees
  - Groove roughness along and across grooves is visible
  - Departures from ideal triangular grooveshape are easily evident
- Left: single groove section of AFM data
- Right: average groove shape and 'best fit' triangle
  - Error bars represent propagated height uncertainty

Groove metrology example - 600/mm red blaze reflection grating





Left: single groove section of AFM data (micron units)
Right: average groove shape and 'best fit' triangle

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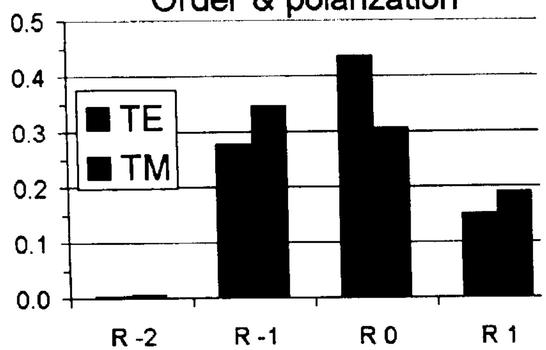
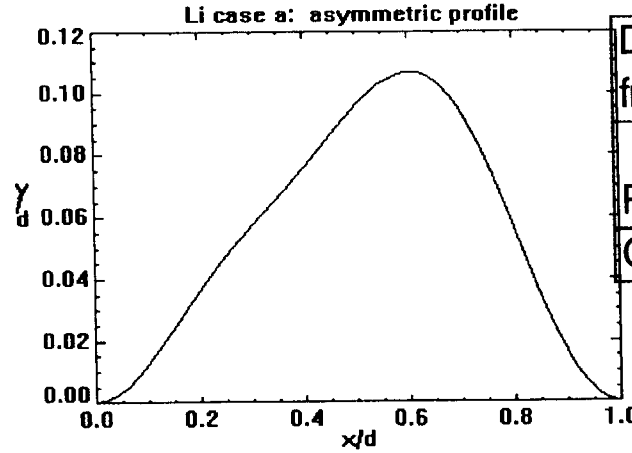
Grating efficiency codes - brief description

- Methods include integral, differential, coupled mode
  - Principal commercially available codes:
    - "Pc Grate" - integral method
    - GSolver - coupled mode method
    - Both of these can model real layer indices, arbitrary (single valued) profiles, transmission & reflection, I.e. realistic cases
  - Proprietary codes used extensively at universities & by companies; examples noted here include:
    - "Delta" - Lifeng Li
  - Other people using coupled modes for this comparison, preliminary results not presented here - thanks to D. Chambers/U. AL Huntsville, C. Raymond/BioRad
  - Figures of merit for any code:
    - energy conservation, stability, execution time
    - Accuracy for known cases - subject of this study

Comparison between Li's results and other codes - 1 of 3 [α=15°, d=2λ for all 3 cases]

- First case - asymmetric profile shallow reflection grating, finite conductivity
  - L: Li's results [L. Li, Appl. Opt. **38**, 304 (1999).]
  - Mid: profile R: Statistics over orders & TE/TM
- Basic result - compared to PcGrate [v. 2000ML] and GSolver [v. xx]
- Fairly good consistency for this case, but rms difference between GSolver and Delta is > 1%

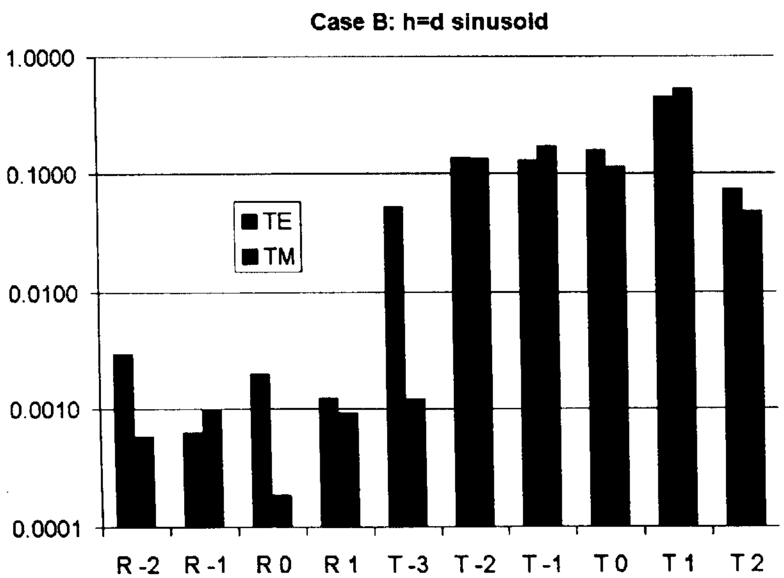


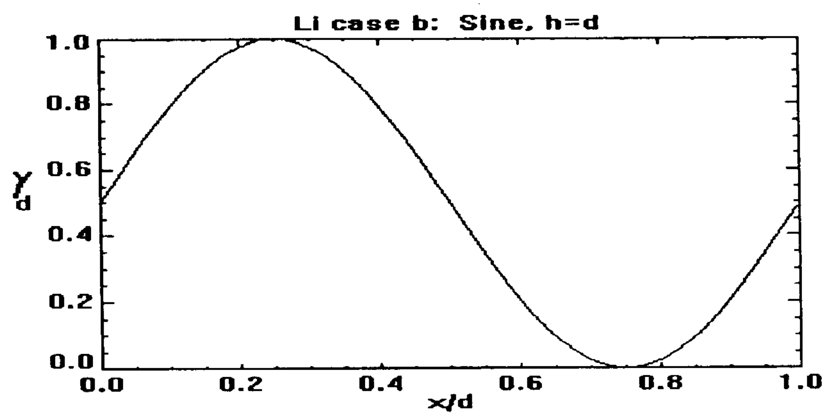


Diff. from Li:	Avg	rms
PcGrate	-0.003%	**0.14%**
GSolver	-1.11%	1.52%

Comparison between Li's results and other codes - 2 of 3

- 2nd case - deep (h=d) sinusoidal transmission grating, perfect conductivity
- L: Li's results; R upper: profile; R lower: statistics over orders & TE/TM
- Basic result - PcGrate & GSolver show good consistency for this case also





Diff. From Li:	Avg	rms
PcGrate 3E	-0.0013%	0.085%
Gsolver	0.0020%	0.028%
Tut3d	0.0020%	0.062%

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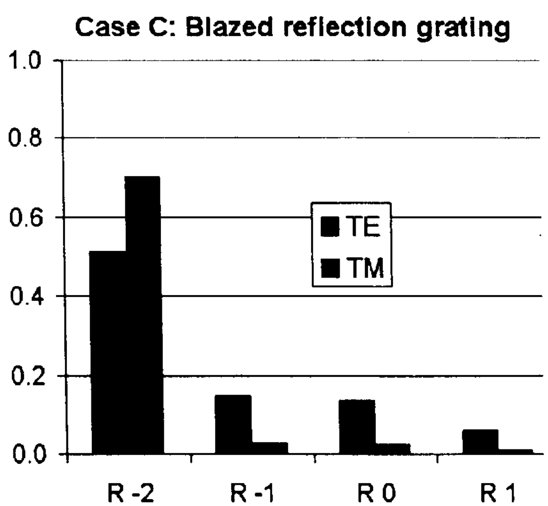
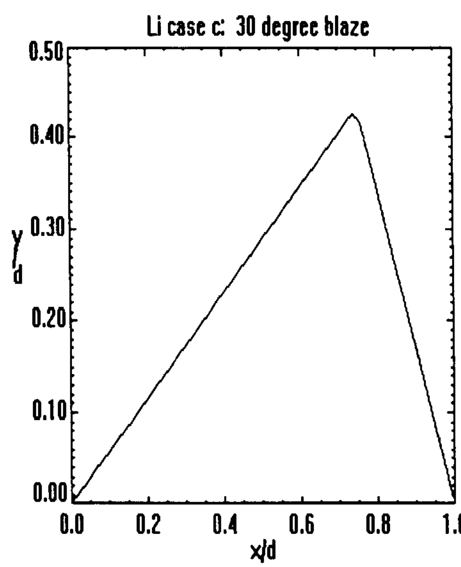
Comparison between Li's results and other codes - 3 of 3

- 3rd case - blazed grating (30° right triangle)
- LL: Li's results; L mid: profile; R- results
- Poor consistency for this case for GSolver
- PcGrate agrees w/ Li's results to w/ in 1%
- 2nd FMM code (TUT3d) also way off





Diff. From Li:	PcGrate	GSolver	Tut3d
R -2 TE	0.06%	0.03%	-0.04%
R -1 TE	0.01%	-0.08%	-0.10%
R 0 TE	-0.05%	-0.12%	-0.15%
R 1 TE	-0.03%	-0.08%	-0.09%
R -2 TM	-0.53%	**-28.35%**	**-22.26%**
R -1 TM	0.17%	-1.11%	1.60%
R 0 TM	0.06%	-2.05%	-1.09%
R 1 TM	0.09%	-0.90%	-0.68%
Avg	-0.03%	-4.1%	-2.9%
rms	0.21%	9.8%	7.9%

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Grating efficiency measurements

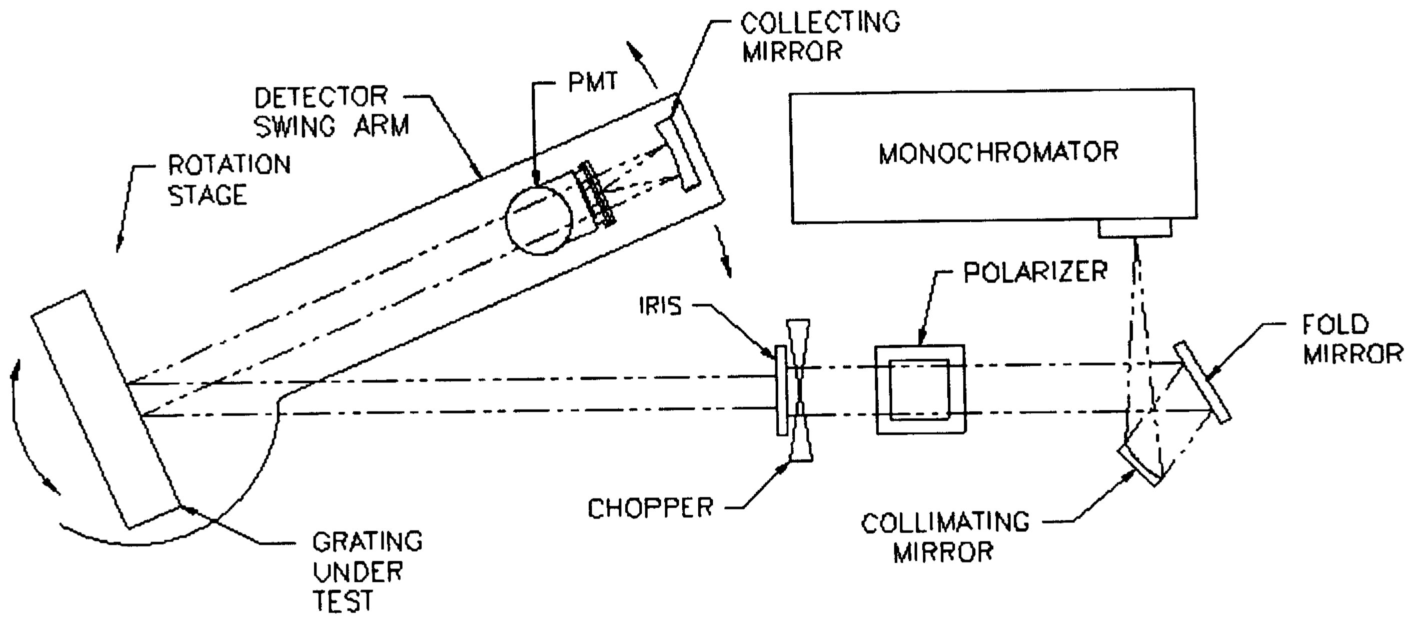

Figure shows Richardson Grating Lab's Automated efficiency checker (AEC), used to measure efficiency from the same gratings whose AFM images were shown

Efficiency comparison

- Definitions:
  - Absolute efficiency is ratio of power in a given order to input power at that wavelength
    - Compare absolute efficiency to values calculated by codes
  - Groove efficiency is absolute efficiency normalized by the reflectance of the coating at the same incident angle

- Cases shown:
  - Red blazed reflection grating 1: n=67/mm, $n\lambda_b \sim 0.05$
  - Red blazed reflection grating 2: n=600/mm, $n\lambda_b \sim 1.25$

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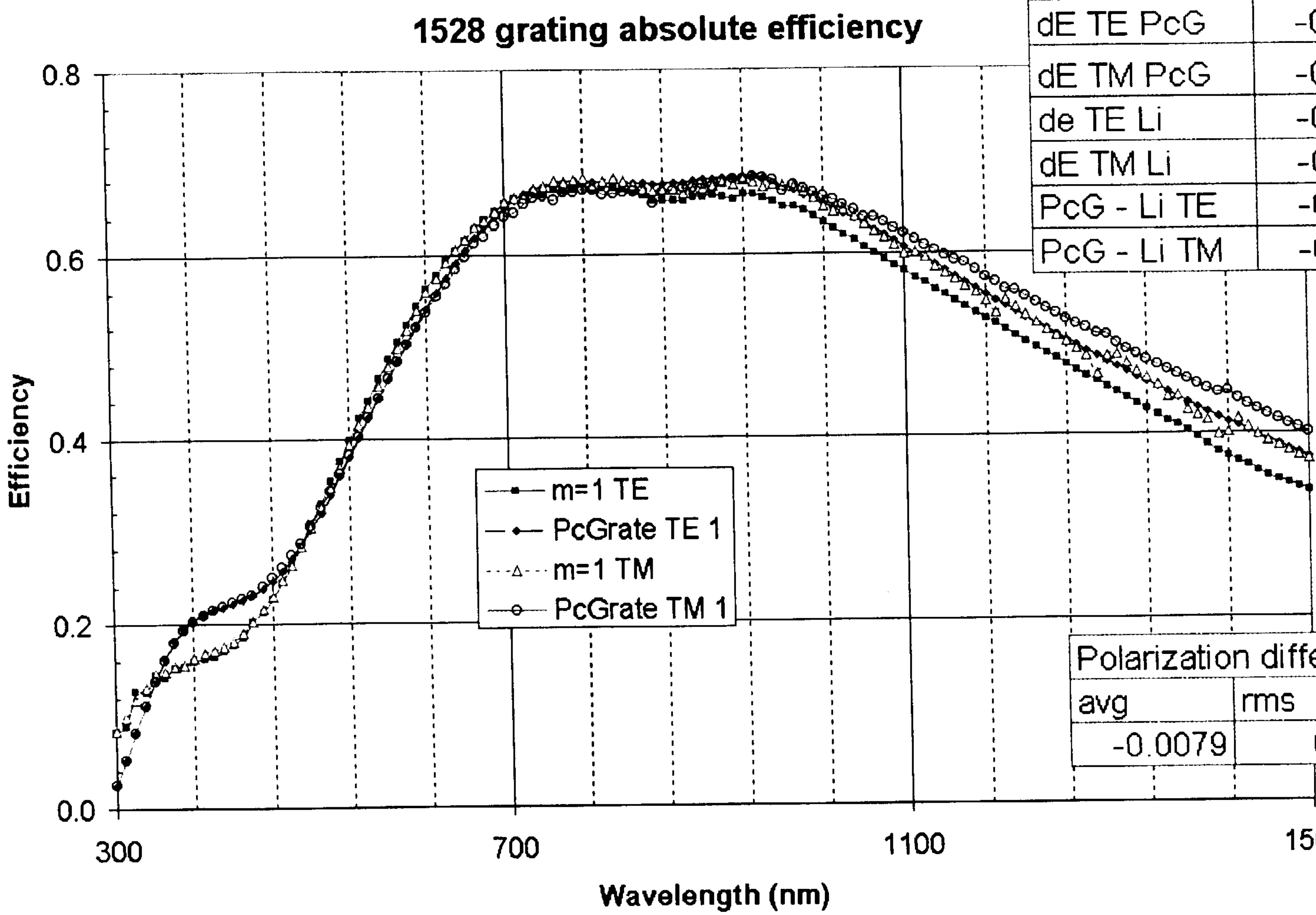
Efficiency comparison 1: 67 groove/mm reflection grating



	avg	rms
dE TE PcG	-0.0009	0.0151
dE TM PcG	-0.0220	0.0306
de TE Li	-0.0031	0.0160
dE TM Li	-0.0232	0.0306
PcG - Li TE	-0.0021	0.0017
PcG - Li TM	-0.0012	0.0039

Polarization difference:

avg	rms
-0.0079	0.0111

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